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Work function of functionalized single-wall carbon nanotubes NICHOLAS SINGH-MILLER, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Engineering the properties of carbon nanotubes is of fundamental importance for many of their practical applications; we focus here on the work function of metallic nanotubes, and on the changes that can be induced by electropositive or electronegative functionalizations. We study with density functional theory pristine, hydrogenated, and fluorinated (5,5) and (5,0) nanotubes along with more complex organic ligands as functional moieties, paying particular attention to the additional dipole interactions that can arise in periodic boundary conditions. Control of the Fermi level alignment is especially relevant for field-effect devices and for the Schottky barrier at carbon nanotube interfaces.

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